

FINAL TECHNICAL/SCIENTIFIC REPORT

1. Award Information

Award Number: DE-FG07-04ID14609

Awardee Name: University of Missouri System, Columbia

Project or Awardee Project ID. 00003521

Project Title: Nuclear Aerosols: Direct Simulation and Elucidation of the Role of Multiple Components, Radioactivity, Charge, Shape and Spatial Inhomogeneity

Principal Investigator: Sudarshan K. Loyalka

Date of Report: October 12, 2008

Period covered by the Report: Jul 15, 2004 - Jul 14, 2008

2. Distribution limitations:

None.

3. Executive summary

Nuclear aerosols can originate from severe core damage in light water reactors, core disruptive accidents in fast reactors, nuclear accidents during nuclear material transport, at waste disposal sites, or explosions. These aerosols evolve under natural transport processes as well as under the influence of engineered safety features. Such aerosols can be hazardous for the equipment inside the reactor, and when leaked into the environment, pose potential risks to the public. Hence, the origin, movement and distribution of these aerosols need to be studied and controlled.

There have been several computer programs that model accident progression in reactor containments. The aerosols evolve processes such as condensation, coagulation, deposition and evaporation. The set of equations used to describe the aerosol behavior mentioned above is non-linear which makes the problem of multi-component aerosol modeling subject to restrictive assumptions and departure from fidelity to actual physics. The purpose of this project was to explore use of the Direct Simulation Monte Carlo (DSMC) technique to elucidate the role of various physical phenomena that influence the aerosol evolution, and eventually help improve computer programs that are used in safety analysis.

The project led to publication of a number of articles in peer reviewed journals that progressively focused on coagulation, condensation, deposition, source reinforcement and that also explored parametric sensitivity of results, and aspects of DSMC sampling processes. Progress was also realized on DSMC simulations of transport of a spatially inhomogeneous aerosol, and computations of rate processes associated with charged (and radioactive particles of arbitrary shapes) towards their use in DSMC computations. Together these results provide insights and tools that will be useful in improving the fidelity of nuclear safety analysis codes to actual physics.

4. A comparison of the actual accomplishments with the goals and objectives of the project.

The project was directed at exploring DSMC simulations to improve understandings of multi-component aerosol evolution under processes such as coagulation, deposition, condensation, source reinforcement etc, and the roles of spatial inhomogeneity, particle charge (including self charging because of radioactivity) and shape. The accomplishments are consistent with project goals.

A number of articles were published in the peer reviewed journals (Nuclear Technology and Annals of Nuclear Energy) that progressively focused on coagulation, deposition, condensation and source reinforcement of multicomponent and explored parametric sensitivity of results, and also aspects of DSMC sampling processes. Two new ways of collisional sampling were postulated, and were found to be very effective in improving computational efficiency of the simulations and the number of particles that could be simulated. In some of the simulations it was possible to consider up to about 400,000 particles and 8 different compositions over a wide range of particle sizes. These results have very clearly established that for multi-component aerosols use of approximations that homogenize certain component properties (e.g. density) in computation of aerosol processes such as coagulation can lead to considerable departure from fidelity to actual physics of the phenomena, and they also pave the way for further exploration of the DSMC technique for future applications.

Progress was also realized on DSMC simulations of transport of a spatially inhomogeneous aerosol, and computations of rate processes associated with charged (and radioactive particles of arbitrary shapes) towards their use in DSMC computations.

Three additional manuscripts relating to the above work are in preparation, and these will be submitted to appropriate journals in the post award period.

5. Summary of project activities for the entire period of funding:

The project activities included graduate student recruitment, advisement, research associated with the project, preparation of journal articles, presentations and discussions at technical meetings, and periodic reports to the sponsor.

The project has resulted in a number of technical articles in peer reviewed journals (Nuclear Technology and Annals of Nuclear Energy) that progressively focused on coagulation, deposition, condensation and source reinforcement of multi-component and explored parametric sensitivity of results, and also aspects of DSMC sampling processes. Progress was also realized on DSMC simulations of the transport of a spatially inhomogeneous aerosol, and computations of rate processes associated with charged (and radioactive particles of arbitrary shapes) towards their use in DSMC computations. This work is being continued in the post-award period, and three additional manuscripts are in preparation.

6. Publications (Journal Articles):

Palaniswaamy, Geethpriya; Loyalka, Sudarshan K. Direct simulation Monte Carlo aerosol dynamics: coagulation and collisional sampling. *Nuclear Technology* (2006), 156(1), 29-38.

Palaniswaamy, Geethpriya; Loyalka, Sudarshan K. Direct simulation Monte Carlo aerosol dynamics: collisional sampling algorithms. *Annals of Nuclear Energy* (2007), 34(1-2), 13-21.

Palaniswaamy, Geethpriya; Loyalka, Sudarshan K. Direct Simulation, Monte Carlo, multicomponent, aerosol dynamics: coagulation, deposition, and source reinforcement. *Nuclear Technology* (2007), 160(2), 187-204.

Palaniswaamy, Geethpriya; Loyalka, Sudarshan K. Direct simulation, Monte Carlo, aerosol dynamics: Coagulation and condensation. *Annals of Nuclear Energy* (2008), 35(3), 485-494.

These are peer reviewed articles, and are available in the public domain. Summaries related to the above work were presented and were also published in contemporaneous Transactions of the American Nuclear Society. These summaries are also in the public domain.